Adaptive Integration

Sunday, October 11, 2020 5:39 PM

This is ch 4.6 in $\underbrace{\text{Burden + Faires}}_{\text{Alg. 4.3 is hard to follow}}$, but we'll follow ch 5.7 in Driscoll and Braun

Idea:

Software packages (Mathematica's NIntegrate
Matlab's integral (vs "trapz")
Python's scipy.integrate.quad)
are not going to ask the user for # nodes,
instead they're going to ask for an accuracy (w/ a sensible default)

How can we do this?

Key Mathematical idea: a posteriori error estimate

"a priori" vs "a posteriori" come up a lot in other subjects too, so let's review them:

a priori = estimate before you've done work

+ always valid
− may require knowledge you don't have
− can't exploit it when you get lucky, i.e., it's always pessimistic

Ex: Simpson's Rule

$$\int_a^b f(x)\,dx = \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2) \right) - \underbrace{\frac{h^5}{90} f^{(4)}(\xi)}_{\text{our "a priori" error estimate}}$$

for some $\xi \in (a,b)$, $h = \frac{b-a}{2}$

a posteriori = estimate after you've done work

+ sometimes easier, sometimes more useful (no unknown things involved)
+ can adapt to your specific situation, and it takes it into account if you got lucky
− not useful for prediction or planning, only useful for verifying / certifying
− in some cases (like for our usage in integration) it is a heuristic or based on unverifiable assumptions.

So, let's make an a posteriori error estimate for integration, ie, a practical way to evaluate the error, so we know when we have enough nodes

Start w/ composite Simpson's rule (though you could do a similar derivation for other rules)

Write $S(n)$ to be Simpson's rule w/ n nodes, or $S(h)$

Recall non-composite Simpson has error $-\frac{h^5}{90} f^{(4)}(\xi)$ $\left(h = \frac{b-a}{2}\right)$ $\xi \in (a,b)$

and composite Simpson has error $-\frac{b-a}{180} \underline{h^4 f^{(4)}(\eta)}$ $\eta \in (a,b)$

So composite Simpson's Rule is $O(h^4) = O(n^{-4})$

Apply Richardson extrapolation

$$R(h/2) = S(h/2) + \frac{S(h/2) - S(h)}{15} \quad 15 = 2^4 - 1$$

or

$$R(2n) = S(2n) + \frac{S(2n) - S(n)}{15}$$

Assumption: $R(2n)$ is so much more accurate than $S(2n)$ that the error in $R(2n)$ is negligible, and so

$$E_{\text{error}} = \int_a^b f(x)dx - S(2n) \approx \underbrace{R(2n) - S(2n)}_{\text{our a posteriori error estimate}}$$

$$= \boxed{\frac{S(2n) - S(n)}{15}} = \hat{E}$$

So, basic strategy: double # of n until $|\hat{E}|$ is small.

Details:

① How small should $|\hat{E}|$ be? ie, pick a tolerance "tol" and require $|\hat{E}| < \text{tol}$?

well, it often makes sense to ask for a relative error.

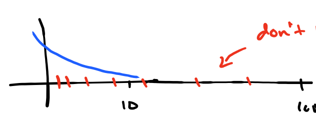
In practice, we usually do both:

Stop when $|\hat{E}| < \text{tol}_{\text{absolute}} + \text{tol}_{\text{relative}} \cdot S(n)$

② Doubling n is going to lead to a lot of nodes very quickly.

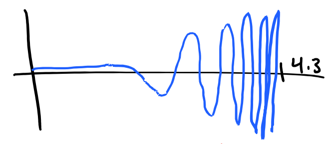
Observation: we often don't need dense nodes everywhere.

Ex: $\int_0^{100} e^{-x} dx$



don't need many nodes here since integrand is so small

Ex: $f(x) = (x+1)^2 \cdot \cos\left(\frac{2x+1}{x-4.3}\right)$



want a lot of nodes here

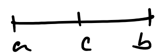
ie., we want to be ADAPTIVE

A nice, popular way to do this is Divide and Conquer (this is a general class of techniques beyond just integration)

Idea:

1) estimate $\hat{E}$ and stop if $|\hat{E}|$ is small enough

2) Split $[a,b]$ in two, $[a,c]$ and $[c,b]$ where $c = \frac{a+b}{2}$



note that $\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx$

Recurse, integrating on $[a,c]$ and estimating its error $\hat{E}_{left}$
and on $[c,b]$ and estimating its error $\hat{E}_{right}$

That's the basic idea.

Usually, we use composite Simpson's rule w/ $n=4$, and are careful to re-use any $f(\text{node})$ computations. See pseudocode

FUNCTION Adaptive Integration ($f, a, b, tol_{abs}, tol_{rel}$)

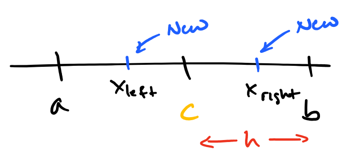
$c = \frac{a+b}{2}$

return $\hat{I}$, nodes = Recursive Integral ($a, f(a), b, f(b), c, f(c)$) // and, implicitly, tol_{abs}, tol_{rel}

FUNCTION Recursive Integral ($a, f(a), b, f(b), c, f(c)$)

$x_{left} = \frac{a+c}{2}$

$x_{right} = \frac{c+b}{2}$



nodes = $\{a, x_{left}, c, x_{right}, b\}$

$h = \frac{b-a}{2}$

$S_2 = h/3\,(f(a) + 4f(c) + f(b))$ // regular (non-composite) Simpson's rule

$S_4 = h/2 \cdot 1/3\,(f(a) + 4\cdot f(x_{left}) + 2\cdot f(c) + 4f(x_{right}) + f(b))$ // composite Simpson

$\hat{E} = 1/15\,(S_4 - S_2)$ // often use 1/10 instead of 1/15 to be more conservative

if $|\hat{E}| < tol_{abs} + tol_{rel}\cdot|S_4|$ // error is acceptable

return S_4, nodes

else // error is too large. So bisect

$\hat{I}_{left}$, $nodes_{left}$ = RecursiveIntegral($a, f(a), c, f(c), x_{left}, f(x_{left})$)

$\hat{I}_{right}$, $nodes_{right}$ = RecursiveIntegral ($c, f(c), b, f(b), x_{right}, f(x_{right})$)

return $\hat{I}_{left} + \hat{I}_{right}$, $nodes_{left} \cup nodes_{right}$ // as lists, the first entry in $nodes_{right}$ is a duplicate of last entry in $nodes_{left}$

end

Summary

All professional integration packages are adaptive so

① they don't waste time where extra nodes aren't needed

② they automatically generate nodes until a tolerance is reached, and give a (heuristic) "guarantee" on the final error.